

Correlations in charged fermion–boson mixture in dimensionalities $D = 2$ and $D = 3$

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Abstract

We numerically study the correlation effects in a two-component charged fermion–boson mixture at zero temperature investigating the role played by the statistical effects and Coulomb correlations in a model with different fermion and boson mass ratios in two and three dimensions. The local-field factors describing the correlation effects and collective excitation modes are determined through the self-consistent scheme. We find that the effects of correlations and statistics are more pronounced in two-dimensional mixtures.

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1. Introduction

The study of exchange and correlation effects in homogeneous two-component system of fermions have been of interest because of applications such as electron–hole liquids in semiconductors [1]. The random-phase approximation [2] (RPA) has been very successful in describing the dielectric properties of the interacting quantum liquids in the high-density limit. As the density of the system is lowered, the exchange and correlation effects become very important. A physically motivated approximation scheme to take the correlations into account is provided by Singwi et al. [3] (STLS) in terms of the local-field factors. The local-field factors take the Pauli–Coulomb hole around a charged particle into account to describe the exchange–correlation effects. A mixture of electrons and charged bosons interacting via Coulomb forces has been considered as a possible model to discuss various properties of high- T_c superconducting materials [4].

In this work we apply the method of Singwi et al. [3] to a mixture of charged fluid of electrons and bosons. There are several motivations to study the two-component (fermion–boson) extension of the self-consistent field approximation. First, Alexandrov and Khmelinin [5] have studied the dielectric properties of a two-component boson–fermion plasma in solid within the RPA. It is of interest to test the validity of RPA and assess the importance of correlation effects through the local-field factors. Second, it was proposed some years ago [6] that for a system of itinerant electrons interacting with local lattice deformations, the crossover regime between adiabatic and non-adiabatic behavior can be described by a model where tightly bound electron pairs of polaronic origin coexist with quasifree electrons with an exchange coupling assumed between them by which bosons can decay into pairs of itinerant fermions and vice versa. It has been suggested [7] that this fermion–boson model can provide a possible scenario for high- T_c superconductivity according to the hypothesis that the fermionic degree of freedom describe holes confined in the copper–oxygen planes, while the bosonic ones are associated with bipolarons which form in the highly polarizable dielectric layers sandwiching the CuO_2 planes. Third, a boson–fermion mixture of atomic gases

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in a trap potential [8] is of recent interest because it provides a testing ground for interaction and statistical effects. Finally, a dilute solution of ^3He atoms in liquid ^4He form a fascinating quantum liquid as an example of interacting fermion–boson mixture [9].

Our basic aim in this work is to investigate the correlation effects in terms of the partial densities and the mass ratio of the respective components within the STLS approximation scheme. The self-consistent field method renormalizes the bare charged potentials to yield reasonable ground state structure factors. We also study the dynamic collective modes in binary liquids.

The rest of this Letter is organized as follows. In Section 2 we outline the formulation of STLS method in application to fermion–boson mixtures. In Section 3 we present our results for the local-field factors, pair-distribution functions and static structure factors. We also analyze the collective excitations of the electron-charged boson mixture within our model. We conclude with a brief discussion and a summary of our numerical results.

2. Theory

We consider a mixture of charged fluid of electrons and bosons as a model system. We assume the system to be at zero temperature, disorder-free, and in the absence of quantizing magnetic field. The interaction between the particles is of long-range Coulomb potential, $v_{\mathbf{q}} = 2\pi(D-1)e^2/q^{(D-1)}$, where D (2 or 3) is the number of spatial dimensions. The system has total density n , and we define the concentrations of individual species as $n_1 = xn$ for electrons and $n_2 = (1-x)n$ for charged bosons, where x is the fraction of fermionic component. We relate the usual coupling strength parameter r_s to the total density n through $r_s a_B = (D/\Omega_D n)^{1/D}$ where Ω_D is the solid angle in D dimension (with $\Omega_2 = 2\pi$ and $\Omega_3 = 4\pi$) and $a_B = \hbar^2 \bar{\kappa}/(\mu e^2)$ being the Bohr radius in which μ is the reduced mass in the system with dielectric constant $\bar{\kappa}$. We also define the mass ratio $\sigma = m_2/m_1$ to allow for different electron and boson masses. The particles are assumed to carry the same charge and the overall charge neutrality is provided by the rigid background.

The multi-component generalization of the STLS theory [10] is based on the linear response theory that the fluctuations in the density of a given component is written as $\delta n_\alpha(q, \omega) = \sum_\beta \chi_{\alpha\beta}(q, \omega) V_\beta^{\text{ext}}(q, \omega)$, where $\chi(q, \omega)$ is the density–density response matrix and $V_\beta^{\text{ext}}(q, \omega)$ is the external perturbing field. In the self-consistent field scheme of Singwi et al. [3] the charge response of the system to an external potential is expressed as

$$\delta n_\alpha(q, \omega) = \chi_\alpha^0(q, \omega) \left[V_\alpha^{\text{ext}}(q, \omega) + \sum_\beta \varphi_{\alpha\beta}(q, \omega) \delta n_\beta(q, \omega) \right], \quad (1)$$

where $\chi_\alpha^0(q, \omega)$ is the response of the non-interacting α th component in general dimension $D = 2$ or 3 [11]. Combining the above equations, we obtain the static STLS expression for the density–density response function of the multi-component sys-

tem

$$\chi_{\alpha\beta}^{-1}(q, \omega) = [\chi_\alpha^0(q, \omega)]^{-1} \delta_{\alpha\beta} - \varphi_{\alpha\beta}(q). \quad (2)$$

Here $\varphi_{\alpha\beta}(q) = v_{\mathbf{q}}[1 - G_{\alpha\beta}(q)]$ are the effective interactions in terms of the static local-field factors $G_{\alpha\beta}(q)$. From the STLS scheme that the two-particle distribution can be decoupled as a product of two one-particle distribution functions multiplied by the pair-distribution function [3] $g_{\alpha\beta}(r)$, the integral expressions for $G_{\alpha\beta}(q)$ involve the static structure factors $S_{\alpha\beta}(q)$ in D dimension

$$G_{\alpha\beta}(q) = -\frac{1}{\sqrt{n_\alpha n_\beta}} \int_0^\infty \frac{d\mathbf{k}}{(2\pi)^D} \frac{\mathbf{q} \cdot \mathbf{k}}{q^2} \frac{v_{\mathbf{k}}}{v_{\mathbf{q}}} [S_{\alpha\beta}(|\mathbf{k} - \mathbf{q}|) - \delta_{\alpha\beta}]. \quad (3)$$

In the above expression for $G_{\alpha\beta}(q)$, the static structure factors $S_{\alpha\beta}(q)$ are related to the density–density response functions by the fluctuation–dissipation theorem

$$S_{\alpha\beta}(q) = -\frac{1}{\pi \sqrt{n_\alpha n_\beta}} \int_0^\infty d\omega \chi_{\alpha\beta}(q, i\omega), \quad (4)$$

where we have used the analytic continuation of the density–density response function to the complex frequency plane followed by the Wick rotation of the frequency integral [2].

Since the local-field factors depend on the static structure factors within the STLS scheme, and the latter depend on the former through the fluctuation–dissipation integral, they have to be calculated self-consistently. Note that when local-field factors are neglected we recover the random-phase approximation results.

3. Results and discussion

We start to solve the STLS set of equations, Eqs. (2)–(4) by repeating until self-consistency is achieved. We have calculated in this way the static partial structure factors $S_{\alpha\beta}(q)$ and the local-field factors $G_{\alpha\beta}(q)$, for various values of density parameter r_s , fermion fraction x , and mass ratio σ . We find that it becomes quite difficult to obtain a self-consistent solution in the STLS scheme, which is based on the dielectric theory, beyond a critical value of r_s in two-component systems. The difficulty for obtaining a self-consistent solution is related to the instability of the system. This instability is due the fact that the local-field factors induce an extra pole in the density–density response function which may or may not be physical. It appears in the large coupling constant region and ultimately the scheme does not converge. As more sophisticated approaches such as the hypernetted chain approximation are free from such instabilities, we surmise that it is a drawback of the STLS scheme rather than anything of physical significance. In the region of r_s values where we can obtain a solution STLS yields reliable results for the importance of correlation effects.

We first present our results for a 3D system. Fig. 1 shows the local-field factors $G_{\alpha\beta}^{\text{3D}}(q)$ in a 3D boson–fermion mixture as a function of $qr_s a_B^*$ for $x = 0.5$, at different r_s and σ values.

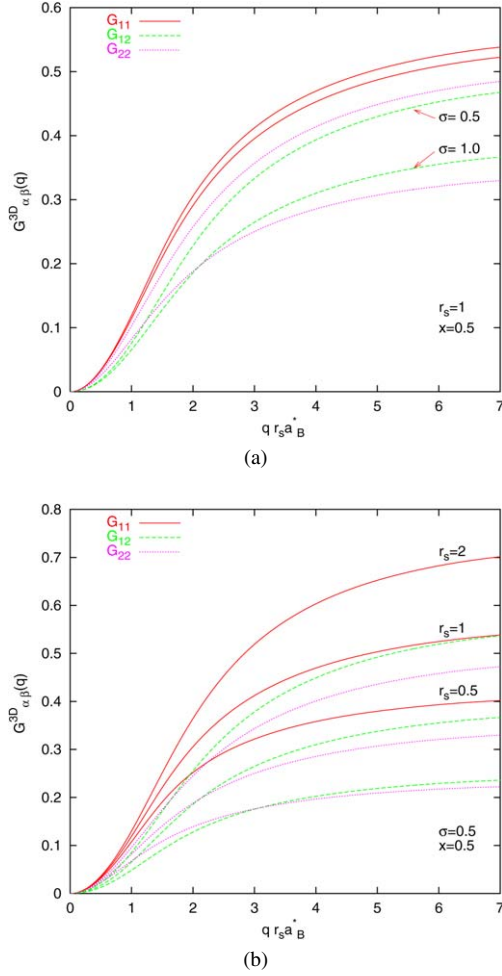


Fig. 1. (Color online.) (a) The local-field factors $G_{\alpha\beta}^{3D}(q)$ in a 3D boson–fermion mixture as a function of $q r_s a_B^*$ for $r_s = 1$, $x = 0.5$, and different values of $\sigma = 0.5$ and 1.0 . The lower curves are for $\sigma = 1.0$. (b) The local-field factors $G_{\alpha\beta}^{3D}(q)$ in a 3D boson–fermion mixture as a function of $q r_s a_B^*$ for $\sigma = 0.5$, $x = 0.5$, and different values of $r_s = 0.5$, 1 , and 2 . The lower curves are for $r_s = 0.5$.

Fig. 1(a) shows the $G_{\alpha\beta}^{3D}(q)$ at $r_s = 1$ and two different σ values. G_{22}^{3D} is more sensitive to the mass ratio σ than G_{11}^{3D} . As σ increases the bosonic particles become more massive and G_{22}^{3D} becomes insignificant. On the other hand, as shown in Fig. 1(b) increasing the r_s value changes the local-field factors more and $G_{\alpha\beta}^{3D}(q)$ in this case are more significant. Since the electron and charged boson densities are the same, the difference between $G_{11}^{3D}(q)$ and $G_{22}^{3D}(q)$ reflect the effects of statistics. In these figures the $G_{11}^{3D}(q)$ are always bigger than $G_{22}^{3D}(q)$ due to the statistics as well.

In Fig. 2 we show the local-field factors in a 2D boson–fermion mixture where the correlation effects are stronger than in 3D systems. Here we have the same physical trends. Because the correlation effects in 2D are in general stronger than in 3D, we observe the degree with which correlations affect different statistics more clearly.

In Fig. 3 we show the partial pair-distribution functions. A precise definition of $g_{\alpha\beta}(r)$ is the probability of finding particle β at distance r away from particle α situated at the origin.

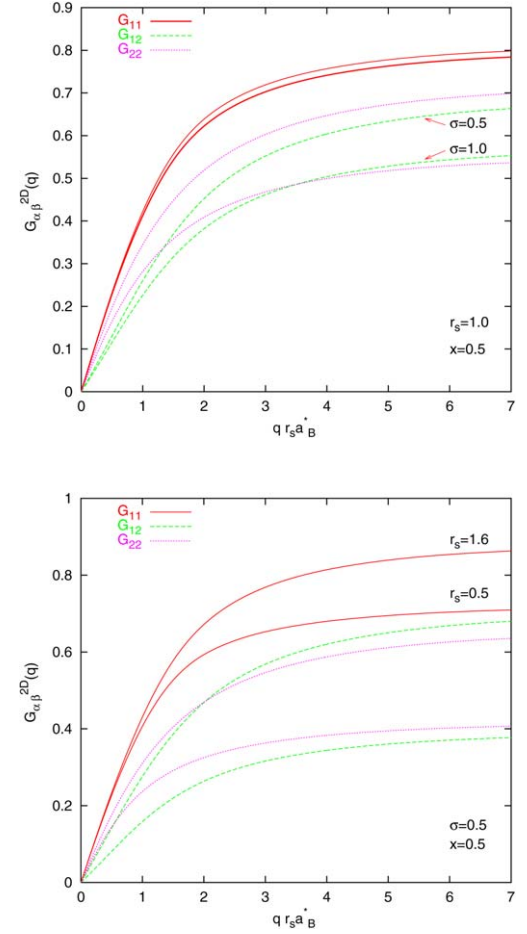


Fig. 2. (Color online.) Top: the local-field factors $G_{\alpha\beta}^{2D}(q)$ in a 2D boson–fermion mixture as a function of $q r_s a_B^*$ for $r_s = 1$, $x = 0.5$, and different values of $\sigma = 0.5$ and 1.0 . The lower curves are for $\sigma = 1.0$. Bottom: the local-field factors $G_{\alpha\beta}^{2D}(q)$ in a 2D boson–fermion mixture as a function of $q r_s a_B^*$ for $\sigma = 0.5$, $x = 0.5$, and different values of $r_s = 0.5$ and 1.6 . The lower curves are for $r_s = 0.5$.

We use the Fourier transform

$$g_{\alpha\beta}(r) = 1 + \frac{1}{\sqrt{n_\alpha n_\beta}} \int \frac{d^D q}{(2\pi)^D} [S_{\alpha\beta}(q) - \delta_{\alpha\beta}] \exp(i\mathbf{q} \cdot \mathbf{r}), \quad (5)$$

to find that $g_{\alpha\beta}(r)$. The first feature to note is that $g_{11}(r)$ becomes smaller with increasing σ and it is understandable because the massive particle has a smaller kinetic energy and the effect of potential becomes more significant. Another fact to note is that with increasing r_s , $g_{\alpha\beta}(0)$ at contact becomes smaller. Moreover, $g_{22}(r)$ at contact tends to one when r_s goes to zero because for a Bose particle the exchange potential is zero due to the absence of Pauli principle.

To indicate the effect of correlations more clearly, in Fig. 4 we show the static structure factor in a 2D mixture of charged fluids in the STLS scheme which takes into account multiple scatterings to infinite order between all components of the plasma compared with the RPA where these effects are neglected. As it is clear from the figure, the value of boson static structure factors are greater than the fermion static structure

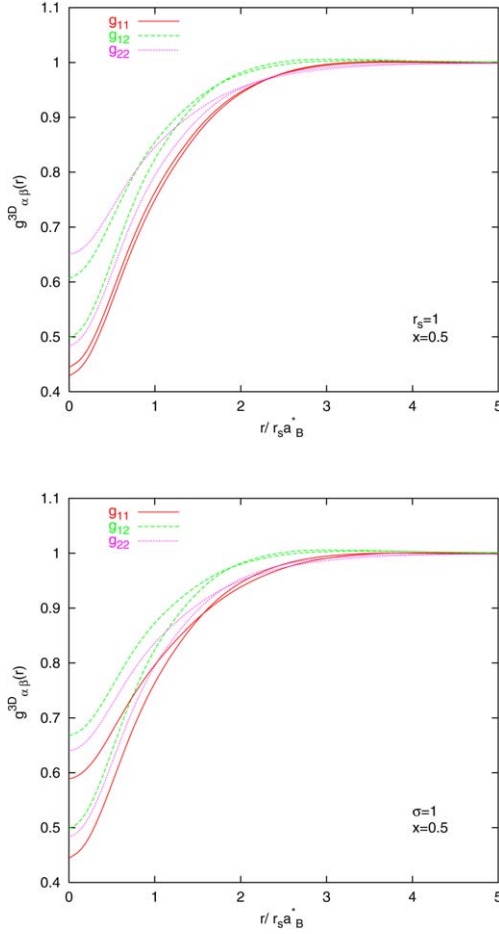


Fig. 3. (Color online.) Top: the pair-distribution functions $g_{\alpha\beta}^{3D}(r)$ in a 3D boson–fermion mixture as a function of $r/r_s a_B^*$ for $r_s = 1$, $x = 0.5$, and different values of $\sigma = 0.5$ and 1.0 . The lower curves are for $\sigma = 0.5$. Bottom: the pair-distribution functions $g_{\alpha\beta}^{3D}(r)$ in a 3D boson–fermion mixture as a function of $r/r_s a_B^*$ for $\sigma = 1$, $x = 0.5$, and different values of $r_s = 0.5$ and 1 . The lower curves are for $r_s = 1$.

factors and then the pair correlation functions for the boson remains above the fermion one at contact. Moreover, with increasing boson mass, the value of static structure factors becomes smaller.

We calculate the collective modes of the mixture by solving for the zeros of the expression

$$\left[\frac{1}{\chi_1^0(q, \omega) - \varphi_{11}(q)} \right] \left[\frac{1}{\chi_2^0(q, \omega) - \varphi_{22}(q)} \right] - \varphi_{12}^2(q) = 0. \quad (6)$$

If $\varphi_{12}(q) = 0$, it can easily be seen that the susceptibility matrix, Eq. (2), becomes diagonal and then two poles of this matrix corresponding to the spectrum of two eigenmodes are separated. We find two discrete modes by calculating numerically Eq. (6) at zero temperature, a branch corresponding to charged bosons (upper curves), and a second branch corresponding to electrons (lower curves). These modes in the small q region (long-wavelength) can be identified as zeroth and second sound or plasmon modes associated with the collective electron and charged boson excitations, respectively, similarly to the case in

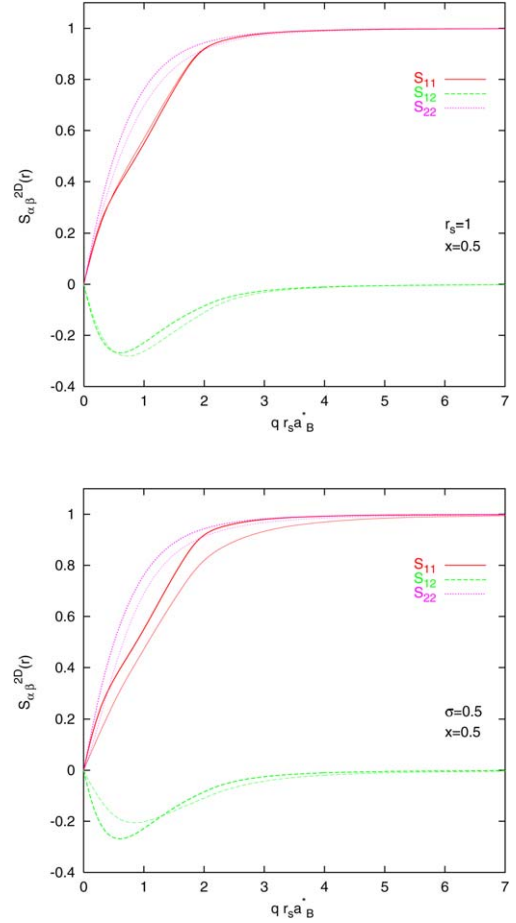


Fig. 4. (Color online.) Top: the static structure factors $S_{\alpha\beta}^{2D}(q)$ in a 2D boson–fermion mixture as a function of $q r_s a_B^*$ for $r_s = 1$, $x = 0.5$, and different values of $\sigma = 0.5$ (thick lines) and 1 (thin lines). Bottom: the static structure factors $S_{\alpha\beta}^{2D}(q)$ in a 2D boson–fermion mixture as a function of $q r_s a_B^*$ for $r_s = 1$, $x = 0.5$ and $\sigma = 0.5$ showing a comparison between the STLS (thick lines) and RPA (thin lines).

^3He – ^4He mixtures in 3D [12]. The spectrum turns out to have a sound-like branch with linear dispersion $\omega \approx c_D v_F q$ in D dimension. Here v_F is the Fermi velocity and the c_D for purely Coulombic interactions and in the high-density limit, is given by $\sqrt{\omega_B^2/\omega_{pl}^2}$ where the boson–plasmon frequency is $\omega_B^2 = \Omega_D n(1-x)e^2 q^\eta/m_2$ and the electron–plasmon frequency of the mixture is given by $\omega_{pl}^2 = \Omega_D n e^2 q^\eta [x + (1-x)/\sigma]/m_1$ with $\eta = \delta_{2,D}$. It is seen that $c_D < 1$ for all concentrations, x and mass ratios σ . This simply means that the electron sound mode lies inside the particle–hole continuum in both 3D and 2D systems.

In Figs. 5 and 6 we show the excitation modes of the system both in 3D and 2D, respectively. An interesting feature to note in these figures is that for small values of σ , the boson mode goes out from the particle–hole continuum area and for the massive boson particle, the mode remains in this region. The same behavior occurs for the modes when the value of r_s increases. In the 2D case, the boson mode goes out of particle–hole continuum area for $\sigma = 0.5$ and up to $r_s = 1.8$.

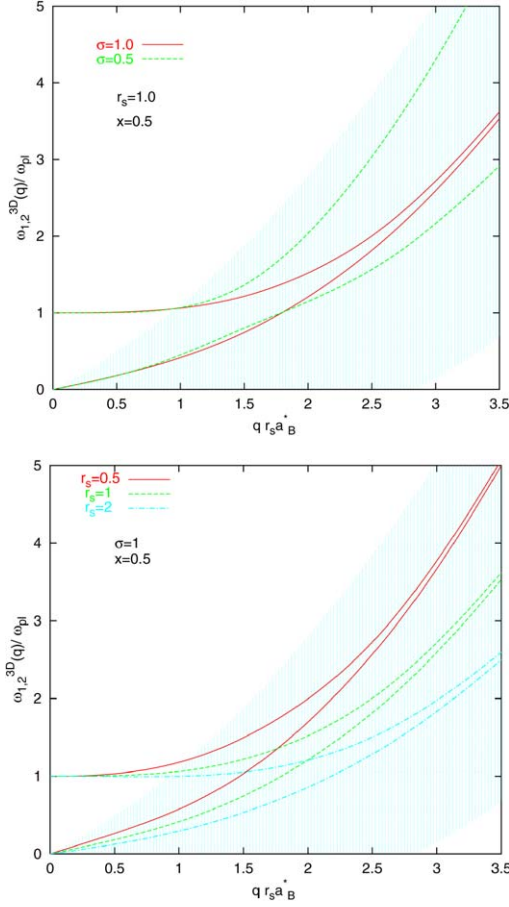


Fig. 5. (Color online.) Top: the collective modes $\omega_{\alpha\beta}^{3D}(q)$ in a 3D boson–fermion mixture in units of $\omega_{pl}(x=0.5) = (2\pi n e^2/\mu)^{1/2}$ as a function of $q r_s a_B^*$ for $r_s = 1$, $x = 0.5$, and $\sigma = 0.5$ and 1.0 . Dotted region denotes the particle–hole continuum. Bottom: the collective modes $\omega_{\alpha\beta}^{3D}(q)$ in a 3D boson–fermion mixture as a function of $q r_s a_B^*$ for $\sigma = 1.0$, $x = 0.5$, and different values of $r_s = 0.5, 1$, and 2 .

4. Concluding remarks

We have presented a study of the correlation effects in a charged electron–boson mixture by performing self-consistent field calculations in two and three dimensions at zero temperature. Correlation effects are found to be strongly dependent on r_s values, electron fraction x and mass ratio σ . Our results are in qualitative agreement with hypernetted-chain approximation calculations [4,13] on a similar system with hole bosons in 3D. We find two discrete collective modes, a branch corresponding to charged bosons and the other corresponding to electrons with linear dispersion in the small q region. Our calculations of the ground state properties of fermion–boson mixture can be extended into several directions. It is straightforward to study the mixture for which the fermion component is spin-polarized or even with partial spin polarization. We have based our calculations on the zero temperature STLS scheme. It should be possible to investigate the finite temperature effects by modifying the response functions of non-interacting particles and fluctuation–dissipation theorem at finite temperature, thereby employing the finite-temperature formalism of STLS.

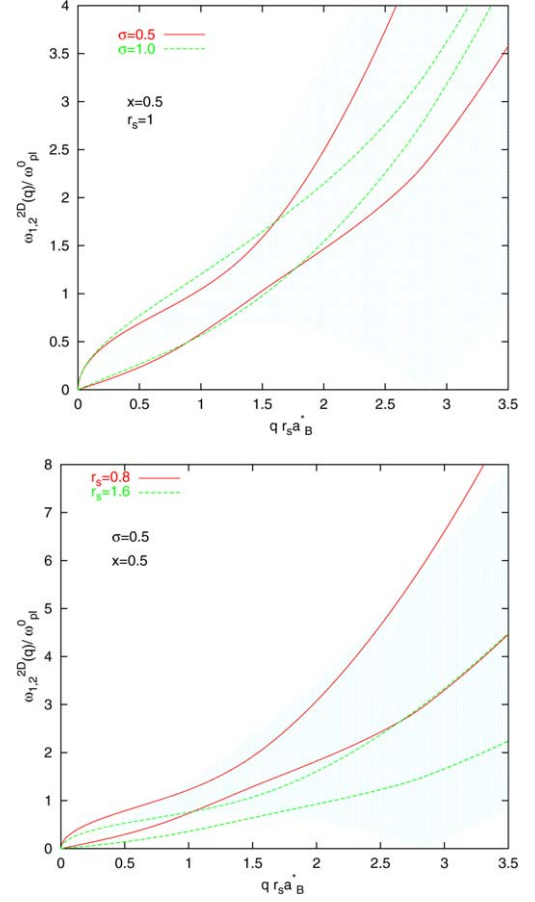


Fig. 6. (Color online.) Top: the collective modes $\omega_{\alpha\beta}^{2D}(q)$ in a 2D boson–fermion mixture in units of $\omega_{pl}^0(x=0.5) = (\pi n e^2/\mu)^{1/2}$ as a function of $q r_s a_B^*$ for $r_s = 1$, $x = 0.5$, and $\sigma = 0.5$ and 1.0 . Dotted region denotes the particle–hole continuum. Bottom: the collective modes $\omega_{\alpha\beta}^{2D}(q)$ in a 2D boson–fermion mixture as a function of $q r_s a_B^*$ for $\sigma = 0.5$, $x = 0.5$, and different values of $r_s = 0.8$ and 1.6 .

Acknowledgements

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